3-Amino-9-ethylcarbazole

132-32-1 | DTXSID1030319

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 119 °C

Global applicability domain: Inside

Local applicability domain index: 5.73e-01

Confidence level: 3.66e-01

Nearest Neighbors from the Training Set

Image not found
3-Amino-9-ethylcarbazole
Measured: 99.0
Predicted: 119

Image not found
Quinoline-2-carbonitrile
Measured: 95.0
Predicted: 89.8

Image not found
Quinoline-3-carbonitrile
Measured: 109
Predicted: 89.8

Image not found
4-cyanoquinoline
Measured: 104
Predicted: 89.8

Image not found
2-Phenylbenzimidazole
Measured: 293
Predicted: 195